Book Review

Reviews in Computational Chemistry, Volume 7. *Edited by Kenny B. Lipkowitz and Donald B. Boyd, VCH Publishers, Inc., New York, 1996, xxiii + 414 pp. ISBN 1-56081-915-4*

This volume will make an excellent addition to the collection of any computational chemist or any scientist who is interested in molecular modeling and computer-aided drug design. It compiles some reviews and tutorials on several different, but important topics in computational chemistry. There are a total of six chapters and an appendix. Two chapters are on searching molecular structure databases, one chapter on methods and applications of combined quantum mechanical and molecular mechanical force fields in statistical mechanical and molecular dynamics simulations, two chapters on density functional theory and its applications, and one chapter on theoretical prediction of vibrational circular dichroism spectra.

The first two chapters are reviews on creating and searching molecular structural databases. In Chapter 1, G. M. Downs and P. Willet described methods for measuring similarity in molecular structures and the similarity searching systems of two- and three-dimensional molecular structure databases. In Chapter 2, A. C. Good and J. S. Mason provided tutorials on searching three-dimensional structure databases and showed how to integrate them with the available computational tools to optimize the rational drug design process. In Chapter 3, J. Gao summarized the methodologies and applications of combined Quantum Mechanics and Molecular Mechanics (QM/MM) potentials in statistical mechanical Monte Carlo and molecular dynamics simulations. Chapters 4 and 5 are reviews of density functional theory which is getting popular very recently in the traditional *ab initio* quantum chemistry community. In Chapter 4, L. J. Bartolotti and K. Flurchick gave an introduction to density functional theory (DFT), and in Chapter 5, A. St.-Amant reviewed the practical aspects of density functional theory and its performance in modeling molecular structure, energies, and vibrational frequencies. In Chapter 6, D. Yang and A. Rauk reviewed the theory and applications of quantum mechanical calculations of vibrational circular dichroism intensities. The Appendix (by Prof. D. B. Boyd) lists more than 2,500 programs for molecular modeling, computational chemistry, *de novo* molecular design, quantitative structure–property relationships, synthesis planning, and other facets of computer-aided molecular science. A brief description of each program is given together with the names, addresses, telephone numbers and electronic mail addresses of the people to contact with the programs. This Appendix is very informative and comprehensive. Any one who wants to track down a computational tool of interest will find this appendix useful.

This volume displays an excellent selection of topics, covering both methodologies and tutorials, of current interest in computational chemistry. The references are excellent, most of them are quite recent. However, there seems a repetition of contents (introduction to density functional theory) in Chapters 4 and 5. This part also appears to be the victim of the time we live in, as the latest development in density functional theory, the hybrid Hartree–Fock/ density functional theory of Becke, is not mentioned in either of the chapters. Recent literature indicates that Becke's hybrid functionals are the most promising among the available functionals. Overall, the chapters are well written and the book is well organized. Anyone who is doing or intend to do computational research on molecular structure and design should seriously consider purchasing this book for his or her personal library.

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J Comput Chem 18:1327, 1997

CCC 0192-8651 / 97 / 101327-01